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Extremal eigenpairs of adjacency matrices wear their sleeves near their hearts: Maximum principles and decay rates for resolving community structure

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Extremal eigenpairs of adjacency matrices wear their sleeves near their hearts

Maximum principles and decay rates for resolving community structure

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ABSTRACT

Understanding relational datasets at a high level is a common data mining task and the detection and classification of community structure is one of the foremost algorithmic challenges of data science. A common approach is to model a dataset with a graph and to use the arsenal of graph mining methods to describe the properties of the data and find desired structure. This arsenal includes many numerical linear algebra techniques. A well-known approach is to calculate a few eigenpairs of a matrix associated with the graph and use the information in the eigenvalues and eigenvectors to find diverse properties of the graph. Often these eigenpairs guide graph optimization processes to more efficient near-optimal solution. For small and quasi-regular graphs, the choice from the buffet of graph-associated matrices is often unimportant as the performance of the technique may not depend much on which graph matrix is employed. However, in large graphs with highly skewed degree distribution, there are several important considerations in this choice. The calculation cost of finding the eigenvectors and the properties that are determined from these eigenvectors both differ dramatically depending which matrix and set of eigenvectors you choose.

We present maximum principles and decay rates demonstrating, for scale-free graphs, the extremal eigenvectors of adjacency matrices are fundamentally different than those related to Laplacian matrices. The results suggest that adjacency eigenpairs could be effectively used to detect community structure of a given density involving many medium-to-high-degree vertices, but that their use is likely inappropriate for locating community structure in the low-degree portions of graphs.

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1. INTRODUCTION

Assume we seek understanding of the topological structure of a large set of relational data. One of the most common types of topological structure sought is community structure, where relatively many connections exist between a small subset of the vertices. The relational data is typically modeled with a graph, $\mathcal{G}$, a collection of m edges between n vertices, and graph algorithms are utilized to partition the graph into subsets, each ideally having many internal connections and few external connections. A commonly utilized and studied approach to accomplish this is using the eigenvectors of a *graph-associated matrix*, which is either sparse with structure related to the graph or a sparse matrix with a low-rank correction. There are several choices of which matrix to use (and hence which eigenvectors). The common sparse matrices are the adjacency matrix [4], combinatorial graph Laplacian [6], normalized graph Laplacian [3], or signless Laplacian [10, 5], while the modularity matrix represents a low-rank correction to the adjacency matrix [11] as does matrix centering that is common in principal component analysis [9]. Given some properties of sought communities it is extremely useful to know which eigenvectors are most likely to detect the structure type of interest, and much is known already. For example, it is well-known that near-bipartite communities are more easily detected with eigenvectors associated with the smallest eigenvalues of the signless graph Laplacian [10, 5] (alternatively, the most negative eigenvalues of the adjacency matrix, or largest eigenvalues of the normalized graph Laplacian). On the other hand, traditional community structure is often detected using eigenvectors associated with the smallest nonzero eigenvalues of the combinatorial graph Laplacian (alternatively, the most positive eigenvalues of the adjacency matrix, or smallest nonzero eigenvalues of the normalized graph Laplacian). In this work we demonstrate some fundamental properties of adjacency eigenvectors for graphs with one vertex of very high degree, namely the energy in these vectors is highly concentrated near the medium to medium-high-degree vertices and are fairly insensitive to prevalent community structure in the low-degree vertices. Our larger goal is to make strides in understanding the eigenspaces of all graph-associated matrices so that we can more effectively aim for certain types of diverse community structure of different type and size.

The eigenvectors of graph-associated matrices also play a critical role in the application and analysis of all numerical linear algebra techniques that one could potentially apply to a graph-associated matrix. The analysis of methods that

solve linear systems using preconditioned iterative solvers rely on understanding approximation properties of combinations of certain eigenvectors. Approaches involving nonlinear systems and constrained optimization also benefit from understanding of the underlying eigenspaces of linearized operators. Reliably knowing how the quality of a numerical solution is related to the quality of a sought graph property is also of high interest. HPC eigensolvers (e.g. Anasazi [1], SLEPc [7]) have been developed for large-scale physics simulation, and the properties of eigenspaces related to scale-free graphs described in this paper need to be considered when using such software for data mining purposes. Our long term goal is to better characterize the properties of eigenpairs of the various data matrices that data miners employ, to further the understanding of the capabilities and limitations of associated with each numerical linear algebra technique and related software.

When $\mathcal{G}$ is *quasi-regular*, meaning the vertices in $\mathcal{G}$ all connect to roughly the same number of other vertices, the choice of which matrix used for finding traditional community structure may not matter much. In this paper, we focus on describing properties of the eigenvectors associated with the most positive and negative eigenvalues of adjacency matrices related to so called *scale-free* graphs. Many graphs associated with real-world data are scale-free, characterized by a skewed degree distribution: a few vertices of extremely high degree (perhaps $\mathcal{O}(n)$), many vertices of intermediate degree, and very many vertices of low degree (perhaps as low as one or two). We demonstrate, through use of local analysis, that a skewed degree distribution implies strong conditions on the adjacency eigenvectors, suggesting what type of structure can be found robustly with these eigenvectors, and what type cannot. The extremal eigenvalues and associated eigenvectors are strongly influenced by the structure surrounding the few vertices of high-degree and medium-high-degree community structure, while being insensitive to community structure involving vertices of low- to medium- degree, even in cases where this is the dominate form of community structure present.

The extremal adjacency eigenvectors are excellent at locating areas of *high edge density*, the portions of $\mathcal{G}$ where the combinatorial explosion of the number of paths of a given length is most extreme. In this sense of density, a large hub is often quite dense, with or without the presence of any community structure.

In [14] and [17], the authors make a curious discovery regarding the extremal adjacency eigenpairs of scale-free graphs. For each vertex in the graph, they build what we refer to as a *spectral coordinate*, a K-dimensional coordinate consisting of the eigenvector values at vertex i for the K extremal eigenpairs (similar to what is commonly done in principal component analysis [9]). Often for real world graphs, these spectral coordinates make up surprisingly simple structure: $\mathcal{O}(K)$ rays emanating from the origin. Sometimes, theses rays are also almost perfectly aligned with the coordinate axes in K-dimensions. These authors demonstrate that most extreme portions of these lines are often related to tightly-knit structure within the graph and suggest that grouping vertices with their associated line will reveal some communities of the graph. In [16], some theoretical work is done to explain one situation where these occur, when the adjacency matrix is well-approximated by a block diagonal matrix. Interestingly, they also provide some perturbation theory connecting the angle of a ray from the coordinate axes and the size of the perturbation from block diagonal. We observe that this is not the only situation where the rays exist, and they commonly arise from having a few vertices of extraordinarily high-degree, possibly with little community structure and large number of off-block-diagonal entries. Extensions of the results in [16] that analyze high powers of adjacency matrices as perturbations of real-valued, block-diagonal matrices are likely to completely explain the rays' angles from the coordinate axes. In Section 2, the maximum principle we present provides an explanation for what types of vertices possibly show up at the tip of these rays. The decay rates demonstrate which vertices have spectral coordinates positioned along the ray and which vertices have coordinates near the origin.

1.1 Adjacency Eigenpairs

Here, we describe the adjacency matrix, its associated eigenpairs, most of the notation necessary throughout the rest of the paper, and few well- and lesser-known simple results demonstrating that the few extremal eigenvalues of the adjacency matrix are dependent on the graph structure around high-degree nodes and not the low-degree portions. We make use of these spectral bounds in the discussion of the results in Section 2, where we demonstrate that most low-degree vertices are poorly represented by these eigenvectors as well.

A relational dataset may be modeled by graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$ with $n := |\mathcal{V}|$ vertices and $m := |\mathcal{E}|$ edges. We focus on *undirected* graphs, where $(i, j) \in \mathcal{E}$ if and only if $(j, i) \in \mathcal{E}$, which are considerably easier for analysis and application of numerical linear algebra techniques due to the symmetry properties of the associated matrices. We assume the graph is *connected*, or any pair vertices can be connected by a sequence of edges where each pair of successive edges share an intermediate vertex. Also, we assume the graph has no *self-loops*, $(i, i) \notin \mathcal{E}$.

The *degree* of vertex $i \in \mathcal{V}$, written d_i, is the number of edges incident to i. For convenience, we order the vertices by the degree in descending order, so that $d_1 = d_{max}$ is the largest degree and $d_n = d_{min}$ is the smallest. The *degree matrix*, $D \in \mathbb{R}^{n \times n}$, is a diagonal matrix with $D_{ii} = d_i$. For large scale-free graphs, often d_{max} is several orders of magnitude higher than d_{min}. Throughout the paper, we assume d_n is very small (one or two) and d_1 is very large (a significant fraction of n) as is the case for many large, scale-free graphs of interest. Let $\mathcal{N}_i$ be the *graph neighborhood* of i, or all vertices j such that $(i, j) \in \mathcal{E}$, and note $i \notin \mathcal{N}_i$ due to assumption that no self loops exist. We have $|\mathcal{N}_i| = d_i$.

For ease of explanation we consider *unweighted graphs*, where each edge has equal weight of 1. The results in this paper easily extend to *weighted* graphs with skewed degree (density) distribution, where degree is redefined to be the sum of incident edge weights. The *unweighted adjacency matrix*, $A \in \mathbb{R}^{n \times n}$, is a binary matrix that has $A_{ij} = 1$ if $(i, j) \in \mathcal{E}$ and $A_{ij} = 0$ otherwise. We have $A = A^t$, due to the graph being undirected. In this work, we focus on discussing the features of A, yet we briefly discuss fundamental differences with other common matrices.

Consider using numerical solution of the following *eigenproblem* for data mining tasks,

$$A\mathbf{w}_k = \lambda_k \mathbf{w}_k$$

for K of the *eigenpairs* $(\lambda_k, \mathbf{w}_k)$, which consist of *eigenvalues* , $\lambda_k \in \mathbb{R}$, and their associated *eigenvectors* $\mathbf{w}_k \in \mathbb{R}^n$. Recall that the symmetry of A implies the eigenpairs are real-valued. The *spectrum* of A, written $\sigma(A)$, is the set of all eigenvalues of A, which has n or fewer members. An eigenvalue is *simple* if it is associated with a one dimensional space of eigenvectors and non-simple if it associated with a higher dimensional eigenspace (spanned by two or more linearly independent eigenvectors associated with the same eigenvalue). We write $w_i^{(k)}$ for the individual entries in $\mathbf{w}_k$.

We order the eigenvalues in $\sigma(A)$ in decreasing order and typically consider computing the K *extremal* eigenvalues,

$$\{\lambda_1, ...\lambda_{K_1}, \lambda_{n-K_2+1}, ..., \lambda_n\}, \text{ for } K_1 + K_2 = K, \quad (1)$$

and their associated eigenvectors. The sign and magnitude of these eigenvalues is important in our discussion in the following section, so we describe some basic results. Peron-Frobenius theory and the connectedness of the graph implies *spectral radius* has properties $\rho(A) = \lambda_1 > 0$ and is a simple eigenvalue and an eigenvector, $\mathbf{w}_1$, associated with λ_1 is all of one sign, $w_i^{(1)} w_j^{(1)} > 0$ for any two $i, j \in \mathcal{V}$. We know $\lambda_n \leq -1$ based on $\lambda_n \leq \langle A\mathbf{x}, \mathbf{x}\rangle / \langle \mathbf{x}, \mathbf{x}\rangle$, where $\mathbf{x}$ is vector with a $+1$ in the i-th slot and a -1 in the j-th slot for any edge (i, j). Additionally, if the graph is not bipartite (not two-cyclic) we also have $\lambda_n > -\rho(A)$, and is not guaranteed simple, otherwise $\lambda_n = -\rho(A)$ and is guaranteed simple. Eigenvectors associated with λ_n are opposite sign across many edges, or for $(i, j) \in \mathcal{E}$ quantity $w_i^{(n)} w_j^{(n)}$ tends to be negative. This property cannot hold at every edge around an odd cycle, yet for the purely bipartite case it does hold for all edges in the graph. The *singular values* of A are related to its eigenvalues in the following way: for each $\lambda \in \sigma(A)$, there exists $\mu = |\lambda| \in \sigma(\sqrt{A^2})$. We order $\mu_k \geq \mu_{k+1}$ and note that μ_k is not necessarily $|\lambda_k|$ (i.e. the most negative eigenvalues are related to some fairly positive singular values).

There is a large body of work regarding the spectral radius of A [4]. We focus on the case of a highly-skewed degree distribution, and develop new eigenvalue bounds for the most positive several eigenvalues. These are not the tightest bounds possible, yet are fairly simple to prove and clearly argue that these eigenvalues are related to the structure surrounding high-degree nodes.

Using fundamental matrix theory, we have several results that relate the extremal eigenvalues to the degrees in the degree distribution. First, by Gershgorin's theorem [8] we know $\sigma(A) \in [-d_{max}, d_{max}]$. Next applying Schur majorization to A^2, and noting that $\text{diag}(A^2) = \text{diag}(D)$, we have a series of inequalities on the singular values of A,

$$\sum_{k=1}^{K} d_k \leq \sum_{k=1}^{K} \mu_k^2, \quad (2)$$

in turn, implying that the magnitudes of the most extremal eigenvalues are, on average, bounded below by the square root of the several highest degrees. We spend the rest of this section demonstrating bounds that are related to (2), yet are related to individual most positive eigenvalues, and in regard to graphs with highly-skewed degree distribution.

For $K = 1$, we have $\lambda_1 \geq \sqrt{d_1}$. So, in general, $\lambda_1 \in [\sqrt{d_{max}}, d_{max}]$. We can show that the lower bound is improved if the neighborhood of a high-degree vertex is highly connected.

Let $\mathcal{G}_i(\mathcal{V}_i, \mathcal{E}_i)$ be the induced subgraph of a vertex and its neighborhood. Formally,

$$\mathcal{V}_i := \{i\} \cup \mathcal{N}_i, \qquad \text{and} \qquad \mathcal{E}_i := \{(j,k) \in \mathcal{E} \text{ s. t. } j, k \in \mathcal{V}_i\}.$$

Let $t_i = |\mathcal{E}_i| - d_i$ be the number of triangles that vertex i participates in and note $t_i \in [0, \frac{d_i}{2}(d_i - 1)]$.

Lemma 1.1.

$$\rho(A) \geq \max_{i \in \mathcal{V}} f(d_i, t_i),$$

where for each $d_i \geq 1$, $f(d_i, t)$ is a monotonically increasing function in $t \in (0, \frac{d_i}{2}(d_i - 1))$ such that

$$f(d_i, 0) = \sqrt{d_i} \qquad \text{and} \qquad f\left(d_i, \frac{d_i(d_i-1)}{2}\right) = d_i.$$

Proof. Pick any $i \in \mathcal{V}$. Let $x_i = 1$, $x_j = a$ for any vertex $j \in \mathcal{N}_i$ and $x_j = 0$ for $j \notin \mathcal{V}_i$. Let $\mathcal{S}_i$ contain all vectors that are zero in $\mathcal{V} \setminus \mathcal{V}_i$ and note that $\mathbf{x} \in \mathcal{S}_i$, independent of a. Then, for any $a \in \mathbb{R}$, we have the bound

$$\begin{aligned} \rho(A) &\geq \max_{\mathbf{z} \in \mathcal{S}_i} \frac{\langle A\mathbf{z}, \mathbf{z}\rangle}{\langle \mathbf{z}, \mathbf{z}\rangle} \\ &\geq \frac{\langle A\mathbf{x}, \mathbf{x}\rangle}{\langle \mathbf{x}, \mathbf{x}\rangle} = \frac{2d_i a + 2t_i a^2}{1 + d_i a^2} \end{aligned}$$

We define

$$f(d_i, t_i) = \max_{a \in \mathbb{R}} \frac{2d_i a + 2t_i a^2}{1 + d_i a^2},$$

where the maximum occurs at

$$a^*(d_i, t_i) = \frac{t_i}{2d_i^2} + \sqrt{\frac{t_i^2}{4d_i^4} + \frac{1}{d_i}}.$$

One can verify that $f(d_i, 0) = \sqrt{d_i}$, $f(d_i, \frac{d_i}{2}(d_i - 1)) = d_i$ and $f(d_i, t)$ is monotonically increasing for $t \in (0, \frac{d_i}{2}(d_i - 1))$. □

Lemma 1.1 is tightened a bit by setting $\mathbf{x}$ as the eigenvector associated with the maximal eigenvalue of the adjacency matrix associated with $\mathcal{G}_i$, but we present this alternative form because it facilitates our discussion. In the case that the maximizing vertex is a hub of degree d_{max} with no triangles, this bound is the same as before, $\lambda_1 \geq \sqrt{d_{max}}$. The bound is increased if there are more triangles. In the case where $\mathcal{G}$ contains a clique of size $(d + 1)$ with $d > \sqrt{d_{max}}$ exists, we have a new bound, $\lambda_1 \geq d$.

Additionally, we can derive a series of bounds for the most positive eigenvalues based on the structure surrounding vertices of largest degree.

Theorem 1.1. *Let $\mathcal{I}_k = \{i_1, i_2, ..., i_k\}$ be any set of k vertices that are 3 hops or greater from each other (an independent set in the two-step graph). Then,*

$$\lambda_k \geq \max_{\mathcal{I}_k} \left[\min_{i \in \mathcal{I}_k} f(d_i, t_i) \right],$$

where for each $d_i \geq 1$, $f(d_i, t)$ is a monotonically increasing function in $t \in (0, \frac{d_i}{2}(d_i - 1))$ such that

$$f(d_i, 0) = \sqrt{d_i} \qquad \text{and} \qquad f\left(d_i, \frac{d_i(d_i-1)}{2}\right) = d_i.$$

PROOF. For each $i \in \mathcal{I}_k$, build a vector $\mathbf{x}_i$ that nonzero only in $\mathcal{V}_i$, has a 1 at vertex i, and a at every vertex $j \in \mathcal{N}_i$, with a chosen to give the highest Rayleigh Quotient as possible (as in Lemma 1.1). Let $\mathcal{S}_k$ be the subspace spanned by $\mathbf{x}_i$ for each $i \in \mathcal{I}_k$. Note that $\mathbf{x}_i^t \mathbf{x}_j = 0$ for $i, j \in \mathcal{I}_k$, with $i \neq j$, due to each vertex in $\mathcal{I}_k$ being 3-hops apart. Set

$$P_{\mathcal{I}_k} = \left[\frac{\mathbf{x}_{i_1}}{\|\mathbf{x}_{i_1}\|_2}, \frac{\mathbf{x}_{i_1}}{\|\mathbf{x}_{i_1}\|_2}, ..., \frac{\mathbf{x}_{i_k}}{\|\mathbf{x}_{i_k}\|_2} \right],$$

with the subscript $\mathcal{I}_k$ dropped for terseness, $P := P_{\mathcal{I}_k}$. We see $P^T P = I$ and $P^T A P$ is a diagonal matrix with $f(d_i, t_i)$ as a diagonal entry for each $i \in \mathcal{I}_k$. Using the Courant-Freidrich-Weyl Theorem [8], we have

$$\begin{aligned} \lambda_k &= \max_{\dim(\mathcal{S})=k} \min_{\mathbf{x} \in \mathcal{S}} \frac{\mathbf{x}^t A \mathbf{x}}{\mathbf{x}^t \mathbf{x}} \\ &\geq \max_{\mathcal{S}_k} \min_{\mathbf{x} \in \mathcal{S}_k} \frac{\mathbf{x}^t A \mathbf{x}}{\mathbf{x}^t \mathbf{x}} \\ &= \max_{\mathcal{I}_k} \min_{\mathbf{y} \in \mathbb{R}^k} \frac{\mathbf{y}^t P^t A P \mathbf{y}}{\mathbf{y}^t P^t P \mathbf{y}} \\ &= \max_{\mathcal{I}_k} \left[\min_{i \in \mathcal{I}_k} f(d_i, t_i) \right]. \end{aligned}$$

□

When the K highest-degree vertices are all 3 hops away from each other, then we know $\lambda_k \geq \sqrt{d_k}$ for $k = 1, 2, ..., K$, and these bounds only increase when these vertices are involved in many triangles. Practically, a series of bounds related to Theorem 1.1 can be produced by sequentially cutting out neighborhoods of the graph and finding (or estimating) the largest eigenvalues of the adjacency matrices associated with the subgraphs.

Similar results can be obtained for bounding most negative eigenvalues from above, however the extra connectivity in each $\mathcal{G}_i$ makes the bounds weaken (i.e. they increase).

The K extremal eigenvalues are typically highly dependent on the vertices of highest degree and the structure surrounding these vertices. Commonly, there are several eigenvalues that are at least the square-root of the maximal degrees. In the next section, we demonstrate that the size of these eigenvalues implies degree-related maximum principles and decay rates for the associated eigenvectors.

2. LOCAL ANALYSIS OF SPECTRAL COORDINATES

The spectral techniques we describe are a simple class of graph embedding techniques from constrained optimization. For each set of extremal eigenpairs of a graph-associated matrix, one can write down a set of constraints and an optimization principal related to the graph structure, which the eigenvectors feasibly optimize. Computationally, these constrained optimization problems are attractive, as high-quality eigensolver packages can be employed. However, several desired features of the embedding are not explicitly provided for in the constraints, nor are they weakly enforced in the optimization functional. Here, we describe this situation for adjacency eigenpairs in the context of graphs with skewed degree distribution and analyze some of the basic features of these eigenpairs using the local relationships implied by the eigenequation, $A\mathbf{w} = \lambda \mathbf{w}$.

We make use of the block representation of K eigenvectors,

$$AW = W\Lambda, \tag{3}$$

where $\Lambda \in \mathbb{R}^{K \times K}$ is a diagonal matrix of the eigenvalues from (1) and the columns of $W \in \mathbb{R}^{n \times K}$ are associated eigenvectors. Again, by symmetry of A, we may assume W is orthogonal, implying $W^t W = I$ and WW^t is a projection onto range(W). Note that $w_i^{(k)} = W_{ki}$, $\mathbf{w}_k = W\mathbf{e}_k$, where $\mathbf{e}_k$ is a cardinal vector in $\mathbb{R}^K$, and the i-th row of W is $W^t \mathbf{e}_i$, where $\mathbf{e}_i \in \mathbb{R}^n$. Vector $W^t \mathbf{e}_i$ is a subset of the *Fourier coefficients* of vertex i with respect to the eigenspaces of A. This an embedding from $\mathcal{V}$ to $\mathbb{R}^K$, which we call the *spectral coordinates* of i with respect to W, or briefly, spectral coordinates, when the eigenvectors we refer to are clear from context. Ideally distances and angles between sets of spectral coordinates $W^t \mathbf{e}_i$ and $W^t \mathbf{e}_j$ help us organize the vertices in an efficient manner using clustering processes or classifiers on these low-dimensional datapoints.

The eigenvectors associated with the most positive eigenvalues maximize

$$\text{trace}(W^t A W) \qquad \text{subject to} \qquad W^t W = I. \tag{4}$$

The optimization function can be rewritten as dot product of spectral coordinates across each edge, $\text{trace}(W^t AW) =$

$$\sum_{k=1}^{K} \sum_{(i,j) \in \mathcal{E}} w_i^{(k)} w_j^{(k)} = \sum_{(i,j) \in \mathcal{E}} \sum_{k=1}^{K} w_i^{(k)} w_j^{(k)} = \sum_{(i,j) \in \mathcal{E}} (W^t \mathbf{e}_i)^t (W^t \mathbf{e}_j),$$

Thus, hueristically, maximizing (4) attempts to place the spectral coordinates of the pair of vertices incident to each edge close in angle and far from the origin. We rewrite

$$\sum_{(i,j) \in \mathcal{E}} (W^t \mathbf{e}_i)^t (W^t \mathbf{e}_j) = \sum_{i=1}^{n} \|W^t \mathbf{e}_i\| \sum_{j \in \mathcal{N}_i} \|W^t \mathbf{e}_j\| C_{ij},$$

where $C_{ij} \in [-1, 1]$ is the cosine of the angle between $W^t \mathbf{e}_i$ and $W^t \mathbf{e}_j$ in $\mathbb{R}^K$. One sees that there is much to be gained by placing the high-degree vertices far from the origin and having the vertices in their neighborhood have the same angle, which is a manifestation of some of the properties observed in [14, 16].

The column-orthogonality constraint $W^t W = I$ normalizes the spectral coordinates, while ensuring that $\pm \mathbf{w}_1$ in all K columns is not a feasible solution (which would put all spectral coordinates on a line through the origin). The constraint distributes the spectral coordinates throughout $\mathbb{R}^K$, although the distribution is often quite poor for scale-free graphs, having a mass near the origin and a few outliers along rays.

The full topology of the graph is required to know exactly where the spectral coordinates lie. However, we demonstrate for adjacency eigenpairs that much is known about the magnitude of spectral coordinates based on approximate eigenvalues and on additional local information, such as a vertex degree and the average degree of the vertices in its neighborhood.

Theorem 2.1. **(Local Analysis for Adjacency Eigenpairs)** *Let W and Λ represent K eigenpairs of A with no*

zero eigenvalues. Then,

$$W^t\mathbf{e}_i = d_i\Lambda^{-1}\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} W^t\mathbf{e}_j\right) \quad (5)$$

PROOF. Starting from Equation (3) and noting that A and Λ are symmetric, gives $W^tA = \Lambda W^t$. Then,

$$\begin{aligned}\Lambda W^t\mathbf{e}_i &= W^tA\mathbf{e}_i = W^t\left(\sum_{j\in\mathcal{N}_i}\mathbf{e}_j\right)\\ &= d_i\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} W^t\mathbf{e}_j\right).\end{aligned}$$

No zero eigenvalue is included in the partial eigendecomposition, so Λ is nonsingular and the result follows. □

This degree-dependent relationship between $W^t\mathbf{e}_i$ and the centroid of the spectral coordinates in $\mathcal{N}_i$ is used to demonstrate a maximum principle and simple bounds on rates of decay as we move away from the maximum.

Theorem 2.2. *Let $(\lambda_k, \mathbf{w}_k)$ be eigenpairs of A with $\lambda_k \neq 0$. We have the following results.*

(i) **(Local Maximum Principle)** *If vertex i is such that $|w_i^{(k)}| \geq |w_j^{(k)}|$ for any $j \in \mathcal{N}_i$, then $d_i \geq |\lambda_k|$. Moreover, if $k = 1$, we have $d_i \geq \sqrt{d_{max}}$.*

(ii) **(Low-Degree Periphery Decay)** *Let $\mathcal{S}_\xi^k$ be the set of all vertices q such that $d_q \geq \xi|\lambda_k|$ for $\xi \in (0,1)$. Assume $j \notin \mathcal{S}_\xi$ is at least s hops from $\mathcal{S}_\xi^k$. Then*

$$|w_j^{(k)}| \leq \xi^s \max_{p\in\mathcal{V}} |w_p^{(k)}|.$$

PROOF. First we prove (i). Looking at the k-th coordinate in Equation (5), we see

$$|w_i^{(k)}| = \frac{d_i}{|\lambda_k|}\left|\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} w_j^{(k)}\right| \leq \frac{d_i}{|\lambda_k|}\left(\max_{j\in\mathcal{N}_i}|w_j^{(k)}|\right).$$

If $|w_i^{(k)}| \geq |w_j^{(k)}|$ for any $j \in \mathcal{N}_i$, then $d_i \geq |\lambda_k|$ holds. For $k = 1$, we consider Equation 2 to see $d_i \geq \sqrt{d_{max}}$.

For (ii), note that a global extrema must also be a local extrema. By (i), the vertex that maximizes the quantity $|w_p^{(k)}|$ must be contained in $\mathcal{S}_\xi^k$ for any $\xi \in (0,1)$. Let $\mathcal{R}_{\xi,s}^k$ be the set of vertices at least s hops away from $\mathcal{S}_\xi^k$. Note that $\mathcal{S}_\xi^k \cup \mathcal{R}_{\xi,1}^k = \mathcal{V}$. Also, for any $s \geq 1$, we have $\mathcal{S}_\xi^k \cap \mathcal{R}_{\xi,s}^k = \emptyset$ and $\mathcal{R}_{\xi,s}^k \supset \mathcal{R}_{\xi,s+1}^k$. For $s = 1$, we see

$$\begin{aligned}\max_{j\in\mathcal{R}_{\xi,1}^k}|w_j^{(k)}| &\leq \frac{d_j}{|\lambda_k|}\left(\frac{1}{d_j}\sum_{p\in\mathcal{N}_j}|w_p^{(k)}|\right)\\ &\leq \frac{d_j}{|\lambda_k|}\max_{p\in\mathcal{V}}|w_p^{(k)}| \leq \xi\max_{p\in\mathcal{V}}|w_p^{(k)}|\end{aligned}$$

For $j \in \mathcal{R}_{\xi,s}^k$, we have $\mathcal{N}_j \subset \mathcal{R}_{\xi,s-1}^k$. Using induction on $s = 2, 3, ...,$

$$\begin{aligned}\max_{j\in\mathcal{R}_{\xi,s}^k}|w_j^{(k)}| &\leq \frac{d_j}{|\lambda_k|}\left(\frac{1}{d_j}\sum_{p\in\mathcal{N}_j}|w_p^{(k)}|\right)\\ &\leq \frac{d_j}{|\lambda_k|}\max_{p\in\mathcal{R}_{\xi,s-1}^k}|w_p^{(k)}| \leq \xi^s\max_{p\in\mathcal{V}}|w_p^{(k)}|,\end{aligned}$$

and we have the result. □

Remark 2.1. **(Discussion of Theorem 2.2 for scale-free graphs)** *We use these results to continue the discussion about what types of graph structure are detected using the techniques in [14, 16]. For spectral coordinates associated with extremal adjacency eigenpairs, our results demonstrate the properties listed below.*

- TIPS OF THE RAYS. *Theorem 2.2(i) demonstrates that the tip of a ray (an eigenspoke) must be at a vertex i such that $d_i \geq |\lambda_k|$. If a sought community does not have a vertex with this property, then it will not be seen as the tip of the associated ray, even if this community is a clique.*

- HIGH-DENSITY STRUCTURE. *The largest hubs, networks of medium-size hubs, large communities, and the vertices in the highest core numbers [2] tend to take on large magnitude spectral coordinates.*

- COMMUNITIES IN THE LOW-DEGREE PERIPHERY. *Theorem 2.2(ii) shows that if sought communities are made up of low-degree vertices are a few hops away from high-degree vertices then their spectral coordinates are close to the origin.*

- RATE OF DECAY. *The result in Theorem 2.2 (ii) is the simplest to prove, as a tighter bound would account for the fact that much of each vertex's neighborhood is at least as far from $\mathcal{S}_\xi^k$ as the vertex itself (and most of the vertices in $\mathcal{R}_{\xi,s}^k$ have much smaller degree than $\xi|\lambda_k|$ for a scale-free graph). The rate of decay is often much faster as one moves away from the maximum value.*

- NUMBER OF HOPS. *Due to the small-world nature of many scale-free graphs, power s may not be very large for much of the graph (common examples place the* average shortest path *in the range of 6 to 20 [12]).*

2.1 Local Analysis for Other Common Graph-Associated Matrices

We briefly demonstrate the difference regarding local analysis of other common graph-associated matrices. These differences play important role in how one uses various graph matrices for data mining and how one might solve linear algebra problems involving graph matrices. We introduce some notation to describe the eigenpairs of various matrices. For matrix $M \in \mathbb{R}^{n\times n}$, we consider the following block eigendecomposition $MV(M) = V(M)\,\Theta(M)$, where $V(M) \in \mathbb{R}^{n\times K}$ is an orthogonalized collection of K eigenvectors of M and $\Theta(M)$ is a $K \times K$ diagonal matrix with the associated eigenvalues on the diagonal. When clear which matrix we mean from context, we merely use V and Θ.

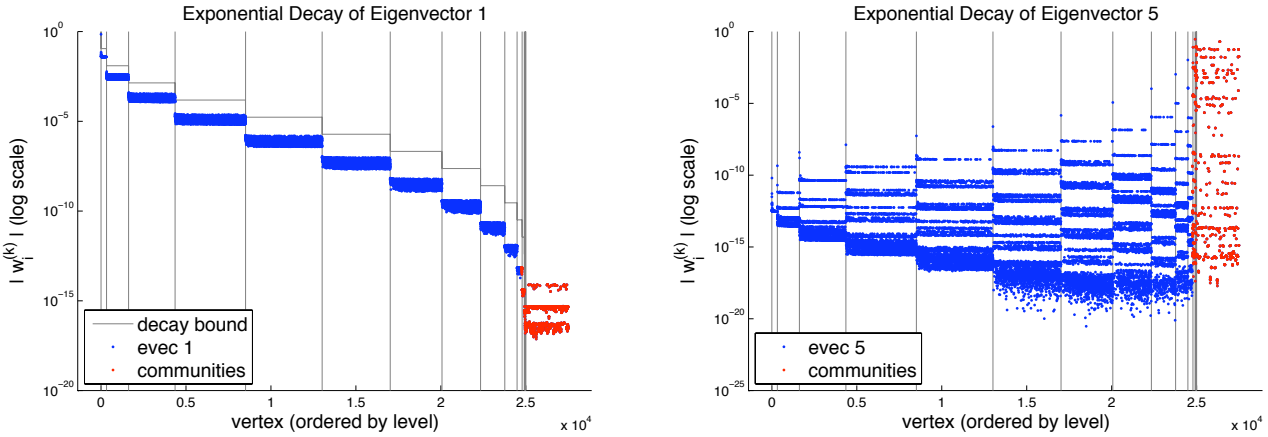

Figure 1: Magnitude for eigenvectors associated with the 1^{st} and 5^{th} most positive eigenvalues for `pattach1`, $c = 11$ and $N = 250$. The vertices from the graph generator are ordered by level (distance from the initial hub), as indicated by the vertical gray lines, and the vertices associated with the community structure are listed last. Red dots represent values associated with community structure. On the left, a decay bound of order $(2/|\lambda_1|)^{\text{level}}$ is plotted to demonstrate that the decay is exponential and related to the size of the eigenvalue, as Theorem 2.2(ii) suggests. On the right we see that the 11-cliques are large enough to be maximums for the fifth eigenvalue, as determined in Theorem 2.2(i).

2.1.1 *Low-Rank Corrections*

Low-rank corrections to A are commonly used in cases of highly-skewed degree distribution. The *modularity matrix*, $B = A - \frac{1}{2m}\mathbf{d}\mathbf{d}^t$, where $\mathbf{d}$ is the vector with d_i in the i-th slot is one example of this. If A_r is a rank-r update to A, the Cauchy Interlacing Theorem [8], implies that the k-th eigenvalue of A_r is bounded below by the $(k+r)$-th of A. Therefore, for scale-free graphs, the most positive eigenvalues are still related to the high-degree vertices and their surroundings. Specifically for B, we see a similar result as Theorem 2.1, allowing us to understand the capabilities associated with the different geometry that these spectral coordinates introduce.

Corollary 2.1. **(Modularity Matrix)** *Let $V = V(B)$ and $\Theta = \Theta(B)$ represent K eigenpairs of B with no zero eigenvalue.*

$$V^t\mathbf{e}_i = d_i\Theta^{-1}\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} V^t\mathbf{e}_j - \mathbf{c}\right)$$

where vector $\mathbf{c} \in \mathbb{R}^K$ is independent of i, and related to a degree-weighted average of all spectral coordinates,

$$\mathbf{c} = \left(\frac{1}{2m}\sum_{j=1}^{n} d_j V^t\mathbf{e}_j\right).$$

Proof.

$$\begin{aligned}
\Theta V^t\mathbf{e}_i &= V^tB\mathbf{e}_i = V^t\left(A\mathbf{e}_i - \frac{1}{2m}\mathbf{d}\mathbf{d}^t\mathbf{e}_i\right)\\
\Theta V^t\mathbf{e}_i &= \left(\sum_{j\in\mathcal{N}_i} V^t\mathbf{e}_j - \frac{d_i}{2m}\sum_{j=1}^{n} d_j V^t\mathbf{e}_j\right)\\
V^t\mathbf{e}_i &= d_i\Theta^{-1}\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} V^t\mathbf{e}_j - \frac{1}{2m}\sum_{j=1}^{n} d_j V^t\mathbf{e}_j\right)
\end{aligned}$$

□

There is still a degree-dependent scale factor present, but the maximum principles and decay properties are quite different. This introduces an interesting geometry, and computing $\mathbf{c}$ provides an advantage in understanding these spectral coordinates. Similar derivations are illustrative for other centered matrices.

2.1.2 *Common Laplacian Matrices*

The local analysis of spectral coordinates associated with the *combinatorial Laplacian*, $L = D - A$, and the *signless Laplacian*, $L_s = D + A$, demonstrates a fundamental difference in the degree-dependence. For small, non-zero eigenvalues less than 1, the associated spectral coordinate of a vertex i is mapped further away from the origin than the centroid of the spectral coordinates in $\mathcal{N}_i$. The smaller d_i is, the further away i's spectral coordinate is from the origin than the centroid (relatively). Therefore the locations of maximums and the decay properties of these spectral coordinates are quite different than those associated with A, tending to map vertices in less-dense parts of the graph further away from the origin.

Corollary 2.2. **(Combinatorial Graph Laplacian)** *Let $V = V(L)$ and $\Theta = \Theta(L)$ represent K eigenpairs of L with no eigenvalue equal to d_i.*

$$V^t\mathbf{e}_i = \left(I - \frac{1}{d_i}\Theta\right)^{-1}\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} V^t\mathbf{e}_j\right)$$

If $\Theta(L)$ has eigenvalues that are all fairly close, then vertex i's spectral coordinate associated with L ends up in nearly the same direction as the centroid of the coordinates corresponding to $\mathcal{N}_i$, whereas the direction is almost the opposite in the case of L_s. In the presence of many odd cycles, this is accomplished by having the spectral coordinates mapped close to the origin.

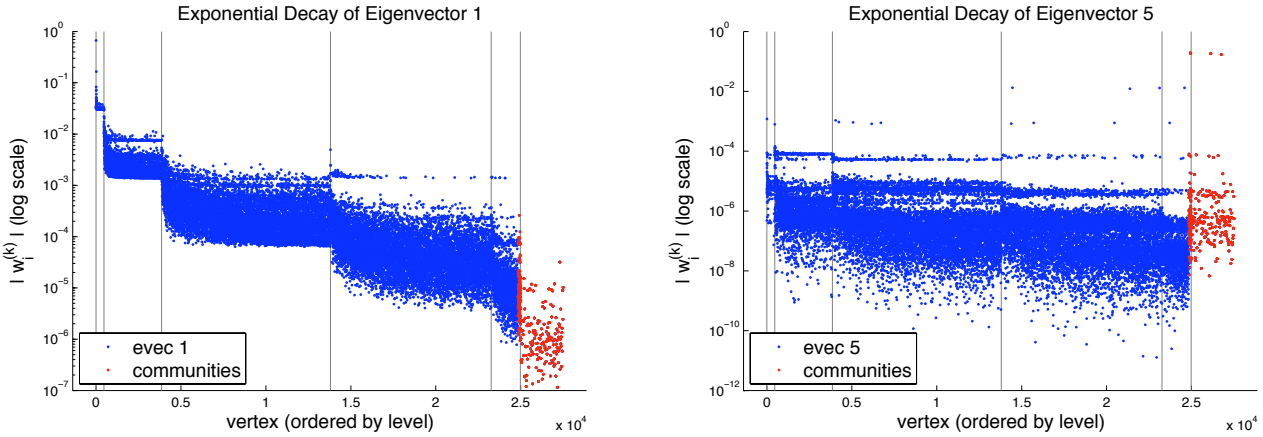

Figure 2: Magnitude for eigenvectors associated with the 1^{st} and 5^{th} most positive eigenvalues for `pattach2`, $c = 16$ and $N = 167$. The vertices from the graph generator are ordered by level (distance from the initial hub), as indicated by the vertical gray lines, and the vertices associated with the community structure are listed last. Red dots represent values associated with community structure. On the left, we see exponential decay as we move away from the vertex of maximal degree. On the right we see that the 15-cliques are large enough to be maximums for the fifth eigenvalue, as determined in Theorem 2.2(i).

Corollary 2.3. **(Signless Graph Laplacian)** *Let $V = V(L_s)$ and $\Theta = \Theta(L_s)$ represent K eigenpairs of L_s with no eigenvalue equal to d_i.*

$$V^t\mathbf{e}_i = -\left(I - \frac{1}{d_i}\Theta\right)^{-1}\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} V^t\mathbf{e}_j\right)$$

One might consider using the high eigenvalues of L and asssociated eigenvectors to find near bipartite structure within a scale-free graph, or the low eigenvalues of L_s and associated eigenvectors to find community structure, due to almost guaranteed rapid convergence of the eigensolver (due to large gaps in the corresponding spectra). The previous two results demonstrate important considerations in this venture. In both cases, using the techniques in Theorem 2.2, we can demonstrate maximum principles centered around high-degree vertices and extremely rapid decay for the vectors associated with the largest eigenvalues of L and L_s. The situation is typically much more severe than the extremal adjacency eigenvectors.

Lastly we demonstrate degree-scaled spectral coordinates related to small nonzero eigenvalues of the *normalized Laplacian* $\hat{L} = I - D^{-1/2}AD^{-1/2}$, which could be thought of as a multiplicative correction to A, have no degree-dependent relationship to the centroid of the (similarly scaled) spectral coordinates associated with vertices in $\mathcal{N}_i$.

Corollary 2.4. **(Normalized Graph Laplacian)** *Let $V = V(L_s)$ and $\Theta = \Theta(L_s)$ represent K eigenpairs of L_s with no eigenvalue equal to d_i.*

$$V^tD^{-1/2}\mathbf{e}_i = (I - \Theta)^{-1}\left(\frac{1}{d_i}\sum_{j\in\mathcal{N}_i} V^tD^{-1/2}\mathbf{e}_j\right)$$

Recall $\sigma(\hat{L}) \in [0, 2]$. Spectral coordiantes associated with eigenvalues near zero are close in direction to the local centroid, whereas the spectral coordinates associated with eigenvalues near 2 are oppposite in direction as the local centroid.

Note that the $D^{-1/2}V$ associated with the smallest non-zero eigenvalues of $\hat{L}$ can easily be shown to be the eigenvectors associated with the most positive eigenvalues of AD^{-1}, the *stochastic propagation operator*.

3. NUMERICAL RESULTS

3.1 Synthetic Graphs

To demonstrate the decay rates and community resolution properties of extremal eigenvectors of A, we embed cliques of various size into graphs from scale-free graph generators that yield graphs with very little community structure. We initialize the graph generator with a small star (a single hub vertex attached to 9 vertices) and then use preferential attachment [15] to introduce new vertices, one at a time, by connecting them to existing vertices with probability proportional to their degree, until we have 25 thousand vertices. The initial hub is highly likely to be the vertex of highest degree when the generation process is complete. As a graph is generated we keep track of each vertice's *level*, or distance from the initial hub vertex, and we use level to order vertices to display the decay properties of extremal eigenvectors. We use two different versions of this generator, `pattach1` and `pattach2`, where each new vertex connects to one or two existing edges, respectively. A graph that is generated by such processed has scale-free degree distribution and is reasonably small in diameter, yet virtually no community structure. Process `pattach1` generates a tree, and `pattach2` generates a graph that is the union of two trees and short cycles are not extremely likely.

After a preferential attachment graph is generated, we attach significant community structure to the vertices furthest away from the initial hub. Specifically, we attach N cliques of size c, each by a single high-level vertex in the generated graph, with N chosen so that roughly 10% of vertices in the final graph are involved in a c-clique. We vary the size of c, recalculate the top several eigenpairs, and investigate the properties of the eigenvalues and associated eigenvectors.

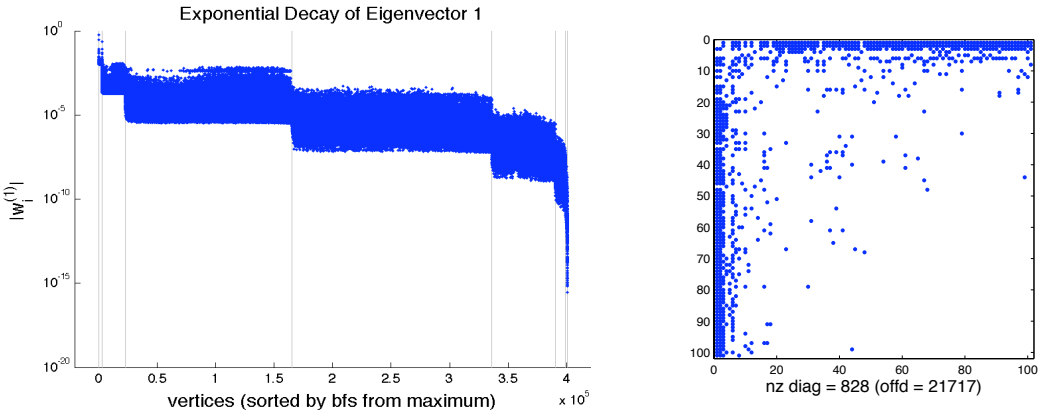

Figure 3: Decay and sparsity plots for real-world example, `amazon0312`.

With this model, we generally observe that when $c << |\lambda_k|$ the k-th eigenvalue is insensitive to the presence of the community structure. Tables 1 and 2 provide a few examples of this phenomenon for `pattach1` and `pattach2` and show how related the eigenvalues are to the square roots of the largest degree.

Additionally, we observe that the clique is only visible to $\mathbf{v}_k$ if the degree of its members is $(c-1) \approx |\lambda_k|$ or larger. We list several examples for `pattach1`. With $c = 6, N = 500$, we do not see the community structure in the extremal adjacency eigenvectors until the eigenvector related to the 77^{th} right-most eigenvalue. For $c = 8, N = 358$, we see the community structure with the 31^{st} eigenpair, for $c = 11, N = 250$, the 5^{th} eigenpair, and for $c = 19, N = 139$, the community structure is present in the right-most eigenpair. We have a similar list related to `pattach2`. For $c = 6, N = 11$, we see no community structure in the 100 right-most eigenpairs. For $c = 8, N = 358$, we see community structure in the 70^{th} eigenpair, for $c = 11, N = 250$, the 19^{th}, for $c = 16, N = 167$, the 5^{th}, and for $c = 22, N = 109$, we see the structure in the 1^{st}. We would need to dig deeper into the spectrum if the community structure were less strong than an clique.

For `pattach1` with $c = 11$ and $N = 250$, the left-hand side of Figure 1 demonstrates the exponential decay of the eigenvector associated with the largest eigenvalue of A, as described in Theorem 2.2(ii). In right-hand side of Figure 1 the the eigenvector associated with the fifth most positive eigenvalue of each adjacency matrix is plotted, where the maximum is obtained on a vertex involved in a clique. This is possible because $(c-1) \approx |\lambda_5|$ and the requirement imposed on a vertex that is a local maximum from Theorem 2.2(i) is satisfied. Figure 2 displays the analogous results for `pattach2` with $c = 16$ and $N = 167$.

3.2 A Real-World Graph

We study `amazon0312`, the undirected version of an amazon product co-purchasing network we downloaded from the SNAP collection [13], which was built by crawling *amazon.com* on March 12^{th}, 2003. Vertices represent products for sale on the website. An edge exists between two products i and j if product$i$ is deemed as frequently bought by the same set of users that bought product j, or vice versa. No self-loops are allowed in the adjacency matrix we use. The

k	$\sqrt{d_k}$	$c = 0$, λ_k	$c = 0$, λ_{n+1-k}
1	+17.8606	+17.9994	-17.9994
2	+12.6886	+12.9172	-12.9172
3	+11.9583	+12.1465	-12.1465
4	+10.7238	+10.7443	-10.7443
5	+10.4881	+10.4183	-10.4183
k	$\sqrt{d_k}$	$c = 11$, λ_k	$c = 11$, λ_{n+1-k}
1	+17.8606	+17.9994	-17.9994
2	+12.6886	+12.9172	-12.9172
3	+11.9583	+12.1465	-12.1465
4	+10.7238	+10.7443	-10.7443
5	+10.4881	+10.4780	-10.4183

Table 1: Eigenvalues of `pattach1`

k	$\sqrt{d_k}$	$c = 6$, λ_k	$c = 6$, λ_{n+1-k}
1	+21.4709	+22.1004	-21.6228
2	+17.7482	+17.8817	-17.9628
3	+15.0333	+15.5960	-15.3273
4	+14.8997	+15.1071	-15.2066
5	+14.3527	+14.6567	-14.6572
k	$\sqrt{d_k}$	$c = 16$, λ_k	$c = 16$, λ_{n+1-k}
1	+21.4709	+22.1004	-21.6228
2	+17.7482	+17.8817	-17.9628
3	+15.0333	+15.5960	-15.3273
4	+14.8997	+15.1071	-15.2066
5	+14.3527	+14.6567	-14.6572

Table 2: Eigenvalues of `pattach2`

graph has $n = 400727$ vertices, and $m = 3200440$ edges. The total number of triangles is 3686467 and average clustering coefficient [12] is 0.4113. Ninety percent of the vertices are contained in a subgraph with diameter 7.7.

We solved for the most positive 15 eigenvalues of A and the associated eigenvectors. In Table 3 we list the top 15 eigenvalues. For each eigenvalue we find a vertex i for which the associated eigenvector is maximized in magnitude too demonstrate that the eigenvectors indicate high-degree structure. We report degree, d_i, number of local triangles, t_i, and the associated local measure from Lemma 1.1, $f(d_i, t_i)$, for vertex i. Note that the vertices are not guaranteed to be three hops away, and some of the assumptions in Theo-

k	λ_k	i	d_i	t_i	$f(d_i, t_i)$
1	56.1956	1	2747	1550	52.9784
2	48.2261	3	2247	1475	48.0624
3	46.5151	2	2249	660	47.7178
4	42.3643	4	1413	1050	38.3385
5	40.9791	5	1282	3118	38.2991
6	39.9788	12	698	2297	29.8640
7	38.4942	23	482	2300	27.1133
8	37.7312	67	333	1946	24.7866
9	37.5905	52	367	1837	24.6497
10	37.3198	9	885	2266	32.3920
11	36.0873	26	469	1402	24.8002
12	34.7883	25	474	1669	25.5056
13	34.4431	42	412	1734	24.8323
14	34.4044	48	379	2005	25.2932
15	34.3602	4	1413	1050	38.3385

Table 3: Eigenvalues for `amazon0312` graph.

rem 1.1 are not met for $K > 1$. On the left side of Figure 3, we plot the eigenvector associated with the rightmost eigenvalue, ordered by breadth-first search away from the vertex of maximal degree. We observe exponential decay as we move away from this vertex. On the right side of Figure 3, we plot the sparsity structure of the subgraph associated with the vertices having 100 largest magnitude values in the eigenvector. While there 828 nonzero entries (414 internal edges) on this block, there are 21717 edges into the rest of the graph. This structure is represented clearly by the extremal eigenvector because of a few high-degree vertices and not because of a strong community.

4. CONCLUSION

We prove properties of extremal eigenvectors for adjacency matrices that are of high importance for understanding the graph mining capabilities of methods that utilize these vectors, and we verify these properties numerically on a few simple examples. Specifically, the size of the associated eigenvalue implies a community must have a certain density to be detected using one of these eigenvectors. These limitations may be very high for many of the communities sought. In this venture we introduce some important analysis approaches that are highly useful for understanding the eigenspaces of any graph-associated matrix, and in turn are of fundamental importance to the analysis any graph-mining method utilizing numerical linear algebra.

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